

Effect of energy deposition modelling in coupled steady state Monte Carlo neutronics/thermal hydraulics calculations

Riku Tuominen

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Outline

- McSAFE project
- Some new Serpent features developed in McSAFE
- Background
- Test case
- Results
- Conclusions and future work

McSAFE project

- EU Horizon 2020 project which aims to develop and validate Monte Carlo based coupled tools for large scale LWR applications
- Final goal to model and validate against measurements:
 - Coupled full core pin-by-pin burnup calculations (German PWR, VVER-1000)
 - SPERT-IIIIE RIA-kind transients
- 12 institutions from 7 different countries
- Codes:
 - MC: Serpent, TRIPOLI, MCNP, MONK
 - TH: SUBCHANFLOW
 - TM: TRANSURANUS

New internal coupling approach

- In the previous internal couplings many standard Serpent routines had to be modified in order to make the coupling work
- Changes not included in the official distribution of Serpent
- Difficult to maintain
- Goal was to improve maintainability and make it easy to couple different types of codes to Serpent internally
- The new implementation relies on a few specific coupling routines executed at specific points of the coupled calculation iteration
- These routines are extended/replaced by the user to initiate the correct calls to the coupled codes

New internal coupling approach

- Implemented coupling routines:
 - InitInternal()
 - IterateInternal()
 - TerminateInternal()
 - InternalCouplingSaysStop()
- In addition routines to provide access to Serpent data such as:
 - void GetInterfacePowerArrayByName(char *ifcName, double **P_arr, long *nCells)
 - double GetPresentTime() :
- New input-card "intcoupling" to provide additional parameters to the coupled solvers

Multi-level meshes for pin lattices inside assembly lattices

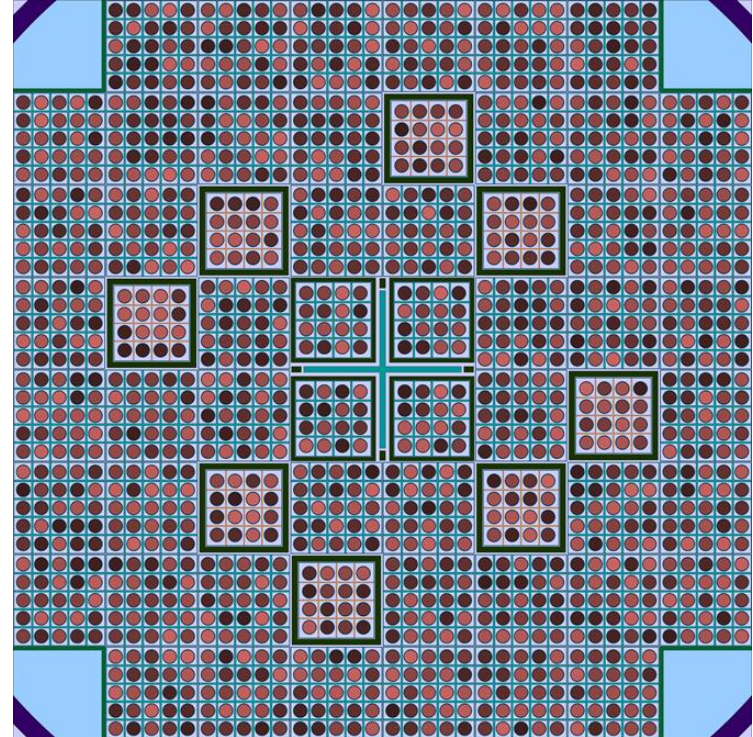
- Previously Serpent has supported regular Cartesian and hexagonal mesh based interfaces
- Pin-level data for assembly-level calculations or assembly-level data for core-level calculations
- Providing pin-level data for core-level calculations is generally not possible using a single regular mesh
- Especially with hexagonal assembly/pin lattices
- Also with square lattices if there are gaps or sleeves between adjacent assemblies
- To tackle these challenges the new interface type allows the user to specify different meshes at different levels of the geometry

SPERT with multi-level meshes

```

22 uo2 2 fuel_power
7
top 1 8 -30.48 30.48 8 -30.48 30.48 1 -1000.0 1000.0
5x5 1 5 -3.71475 3.71475 5 -3.71475 3.71475 1 -1000.0 1000.0
4x4 1 4 -2.9718 2.9718 4 -2.9718 2.9718 1 -1000.0 1000.0
cr1 1 4 -3.2258 2.7178 4 -3.2258 2.7178 1 -1000.0 1000.0
cr2 1 4 -2.7178 3.2258 4 -3.2258 2.7178 1 -1000.0 1000.0
cr3 1 4 -3.2258 2.7178 4 -2.7178 3.2258 1 -1000.0 1000.0
cr4 1 4 -2.7178 3.2258 4 -2.7178 3.2258 1 -1000.0 1000.0
1
nested top 0
5x5 5x5 5x5 5x5 5x5 5x5 5x5 5x5
5x5 5x5 5x5 4x4 5x5 5x5 5x5 5x5
5x5 5x5 4x4 5x5 5x5 4x4 5x5 5x5
5x5 5x5 5x5 cr1 cr2 5x5 4x4 5x5
5x5 4x4 5x5 cr3 cr4 5x5 5x5 5x5
5x5 5x5 4x4 5x5 5x5 4x4 5x5 5x5
5x5 5x5 5x5 5x5 4x4 5x5 5x5 5x5
5x5 5x5 5x5 5x5 5x5 5x5 5x5 5x5

```



Radial temperature distribution

22 UO2 2 fuel_power

2

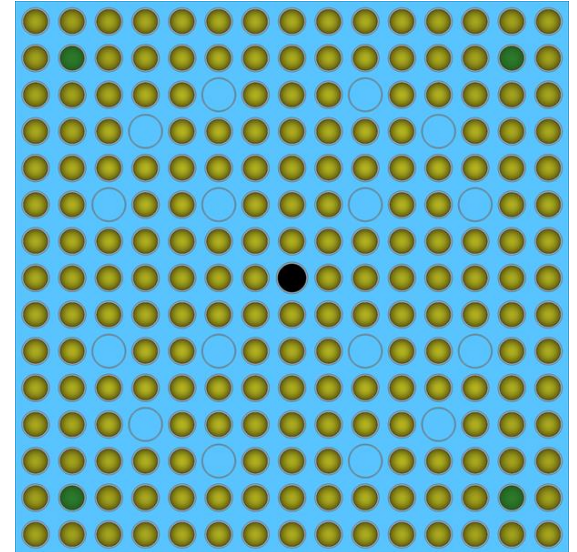
mt 1 15 -10.82025 10.82025 15 -10.82025 10.82025 30 -176.53 176.53

mb 9 10 0.00000 0.05217 0.10433 0.15650 0.20867 0.26083 0.31300 0.36517 0.41733

0.46950

1

nested mt 1 mb



Background

- In the coupled calculations the Monte Carlo code is used to produce a power distribution which in practice means tallying the energy deposition
- Usually the energy deposition has been estimated using an approximate method in which all energy is deposited locally at fission sites
- Goal is to study how the accuracy of energy deposition modelling affects the results of steady state coupled calculations by using
 - internal coupling between Serpent 2 and SUBCHANFLOW
 - different energy deposition modes of Serpent 2
- Focus on light water reactors and as a test case a 3D PWR fuel assembly is modelled

Energy deposition modes

Mode 0

- Default mode used previously in Serpent 2
- All energy is deposited locally at fission sites
- Energy deposition per fission is calculated as

$$E_d = \frac{Q_i}{Q_{235}} H_{235},$$

where Q_i is the fission Q-value for nuclide i , Q_{235} is the fission Q-value for U_{235} and $H_{235} = 202.27$ MeV is an estimate for the energy deposition per fission in a light water reactor

- Spatially inaccurate, magnitude inaccurate

Energy deposition modes

Mode 1

- All energy is deposited locally at fission sites
- Uses ENDF MT 458 data which gives components of energy release due to fission as a function of incident neutron energy
- Energy deposition per fission is calculated as

$$E_d = EFR + ENP + END + EGP + EGD + EB + E_{capt},$$

where EFR is the kinetic energy of the fission products, ENP the kinetic energy of the prompt neutrons, END the kinetic energy of the delayed neutrons, EGP the energy of the prompt gammas, EGD the energy of the delayed gammas, EB the energy of the delayed betas and E_{capt} is an user-defined constant for additional energy released in capture reactions

- Spatially inaccurate, magnitude OK if E_{capt} is OK

Energy deposition modes

Mode 2

- Neutron heating rate is calculated using special microscopic cross sections, expressed in eV·barns, referred as KERMA (Kinetic Energy Release in Materials) coefficients:

$$H(E) = \sum_i \sum_j \rho_i k_{ij}(E) \phi(E),$$

where ρ_i is the number density of material i , $k_{ij}(E)$ is the KERMA coefficient for material i and reaction j at incident energy E , and $\phi(E)$ is the neutron scalar flux at E

- Fission energy deposition is calculated separately based on MT 458 data as

$$E_d = EFR + EGP + EGD + EB$$

- Photon energy is deposited locally at emission sites
- Improved spatial accuracy and magnitude compared to modes 0 and 1 with a small increase in the calculation time

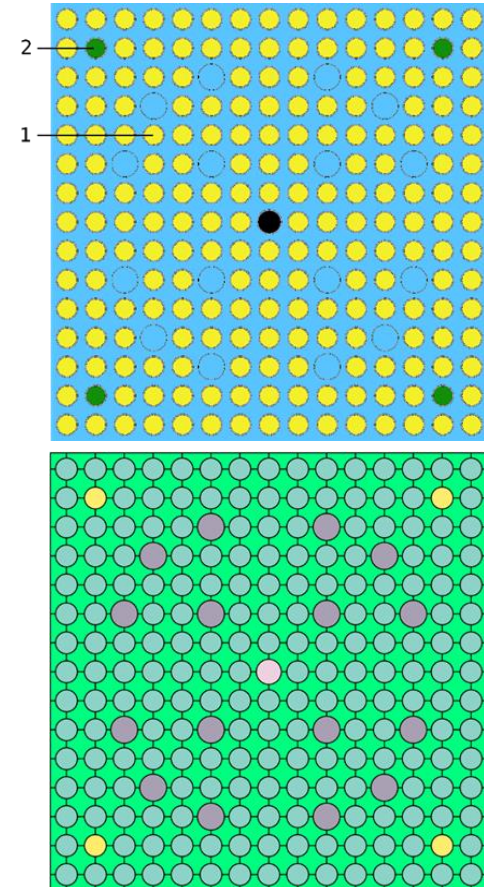
Energy deposition modes

Mode 3

- Adds photon transport to mode 2
- Photons are created during the coupled neutron-photon transport calculation in reactions such as fission, inelastic scattering and radiative capture
- As a simple approximation the energy of the delayed fission gammas is deposited with the same distribution as the prompt fission gammas
- Fission energy deposition is calculated as
$$E_d = EFR + EB$$
- Higher spatial accuracy and computational time compared to mode 2

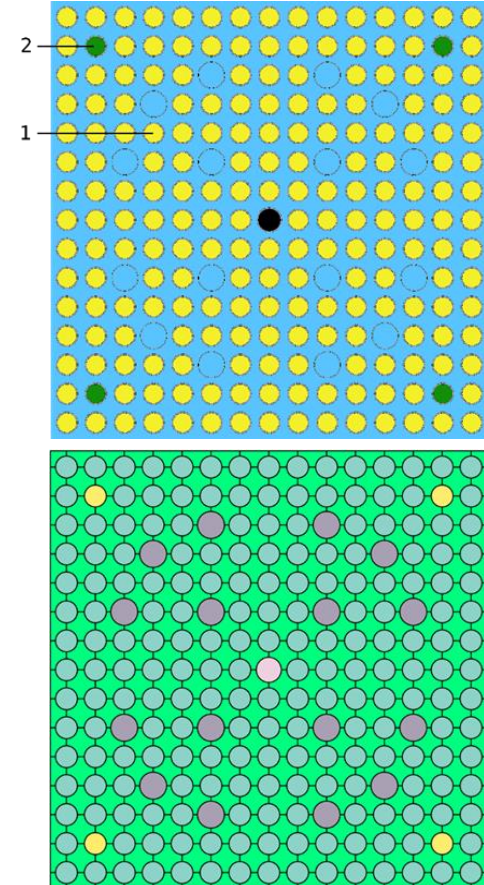
Test case

- 3D 15x15 fuel TMI fuel assembly
- 204 4.85 % enriched UO_2 pins and 4 $\text{Gd}_2\text{O}_3 + \text{UO}_2$ burnable poison pins with fuel enrichment of 4.12 % and Gd_2O_3 concentration of 2 %
- Boron concentration 1480 ppm
- Coolant centered SCF model with 256 channels and 30 axial layers
- Separate multi-physics interfaces for the coolant and the fuel
- Radial temperature profile for each axial layer of each pin was used in Serpent
- Total power in each axial layer of each pin was transferred to SCF

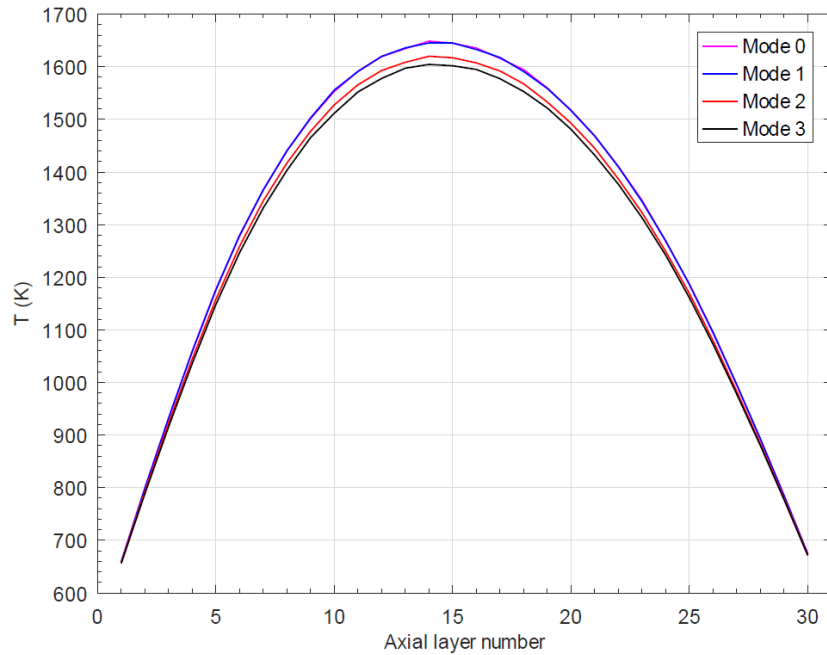


Test case

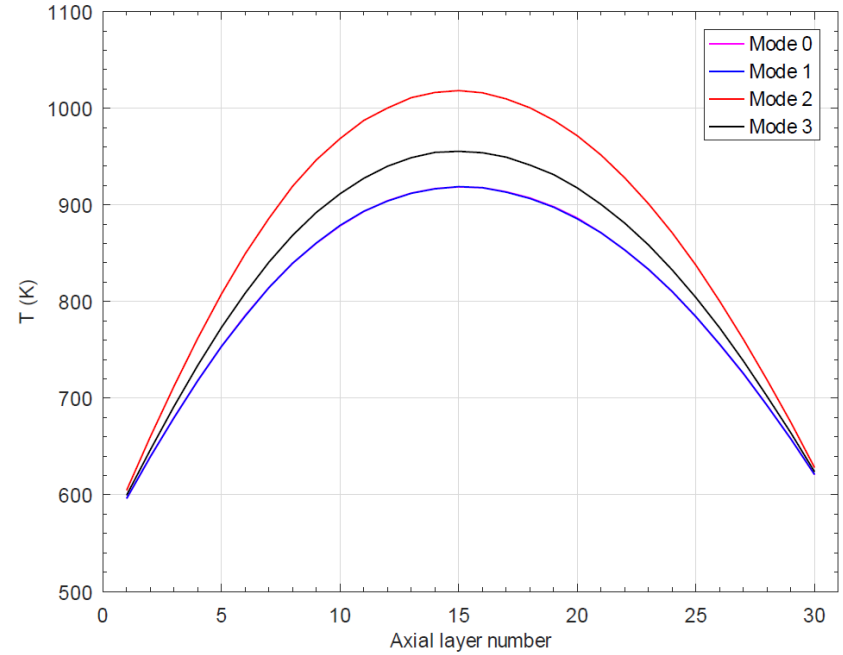
- Separate coupled calculation for each of the energy deposition modes
- 10 coupled iterations in each calculation
- At each iteration 4×10^8 active neutron histories were simulated
- A stochastic approximation based relaxation for the power
- ENDF/B-VII.1 based cross section library was used



Results



Rod 1



Rod 2

Results

Mode	k_{eff}	Calculation time (h)
0	1.23773 ± 0.00003	21.7
1	1.23773 ± 0.00003	21.9
2	1.23793 ± 0.00003	24.5
3	1.23801 ± 0.00003	37.2

Conclusions and future work

- Energy deposition mode has a visible effect on the fuel temperatures
 - Relative differences in the temperatures are larger for the Gd-rods
- Verification/validation of the energy deposition methods is needed
- Burnup calculations
 - The choice of the energy deposition mode defines how the energy deposition used in normalization is tallied
 - Since the tallied average energy deposition per fission differs between the different energy deposition modes so does the fission rate along with other reaction rates

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